

## LA-UR-14-22509

Approved for public release; distribution is unlimited.

Title: IC W13\_auptphase Highlight: Phase Diagram of Pt from Z Methodology

Author(s): Burakovsky, Leonid  
Chen, Shao-Ping  
Preston, Dean L.  
Sheppard, Daniel G.

Intended for: a highlight as part of a report for Institutional Computing program;  
this highlight requires LA-UR number

Issued: 2014-04-15

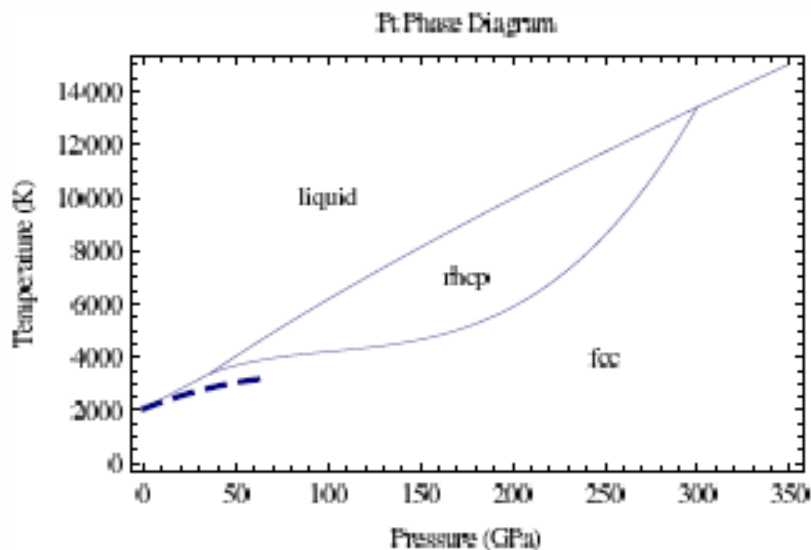


### Disclaimer:

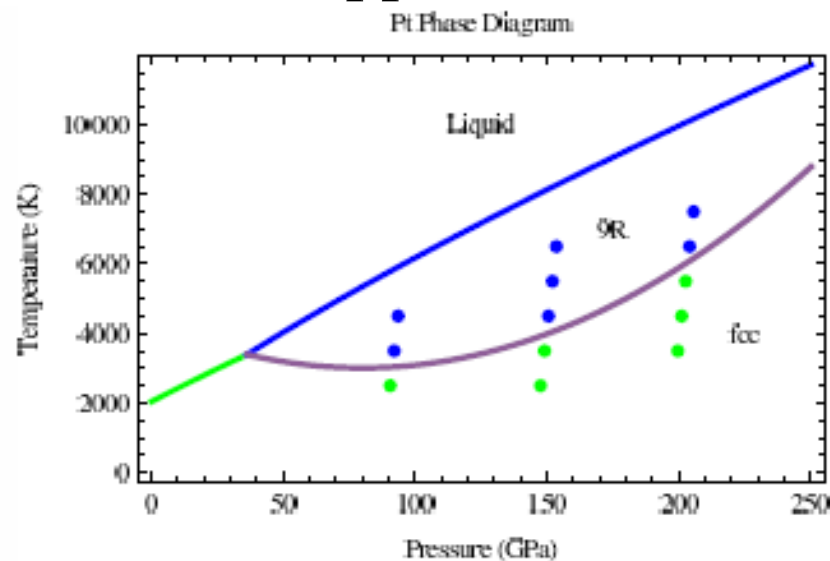
Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

# IC W13\_auptphase Highlight: Phase Diagram of Pt from Z Methodology

**Leonid Burakovsky, T-1 (PI), Shao Ping Chen, T-1,  
Dean Preston, XCP-5, and Daniel Sheppard, T-1**



**Fig. 1.** Pt phase diagram from combining the Z methodology with the fcc-rhcp (face-centered cubic -- random hexagonal close-packed) solid-solid phase boundary. The experimental melting curve of Pt is shown as dashed blue line. Solid-solid phase boundaries in Figs. 1 and 2 are consistent with each other.



**Fig. 2.** Phase diagram of Pt from the Z methodology: fcc-Pt melting curve (green line), liquid Pt solidified into solid fcc (green bullets), 9R-Pt melting curve (blue line), liquid Pt solidified into solid 9R (blue bullets), and the (tentative) fcc-9R solid-solid phase boundary (violet).